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Molecular Dynamics Simulation of High Strain-Rate Void Nucleation in Nanocrystalline Copper.

J. Belak, D.B. Boercker, G.S. Bales, J. Glosli
University of California, Lawrence Livermore National Laboratory, Livermore, CA 94551

Isotropic tension is simulated in nanoscale polycrystalline copper with 10nm grain sizes using large-scale molecular dynamics. The nanocrystalline copper is fabricated on the computer by growing randomly oriented grains from random positions in the simulations cell. Constant volume strain rates of 10^8 - 10^{10} are considered for systems ranging from 10^5 - 10^6 atoms using an EAM interatomic potential for copper. The spacing between voids for room temperature simulations is found to scale approximately as $l \sim 0.005 * C_s/\varepsilon$ where C_s is the sound speed and ε is the strain rate. Below strain rates of about 10^9, only one void is observed to nucleate and grow in the simulation cell. Results are presented for several grain boundary orientations (textures) and compared to macroscopic nucleation and growth models.

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